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6. AUTHOR(S) S. E. Elghobashi, I. Kim, C. H. Chiang, and W. A. Sirignano			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Mechanical and Aerospace Engineering University of California, Irvine Irvine, CA 92717 AFOSR-TR-		8. PERFORMING ORGANIZATION REPORT NUMBER 2 0100	
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**FUNDAMENTAL STUDIES ON DROPLET INTERACTIONS
IN DENSE SPRAYS**

AFOSR GRANT 90-0064

PREPARED BY:

**W. A. SIRIGNANO, PRINCIPAL INVESTIGATOR
S. E. ELGHOBASHI, PROFESSOR,
I. KIM, POSTDOCTORAL RESEARCH ASSOCIATE
C. H. CHIANG, POSTDOCTORAL RESEARCH ASSOCIATE**

**DEPARTMENT OF MECHANICAL AND AEROSPACE ENGINEERING
UNIVERSITY OF CALIFORNIA, IRVINE**

SUBMITTED TO: J. M. TISHKOFF

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FUNDAMENTAL STUDIES OF DROPLET INTERACTIONS IN DENSE SPRAYS

ABSTRACT

Computational studies of interactive, vaporizing droplets have been made in order to understand better the dynamics of dense sprays. Axisymmetric situations with droplets moving in tandem and three-dimensional situations with droplets moving in parallel have been considered. Detailed velocity and thermochemical properties fields have been determined. Lift and drag coefficients, Nusselt numbers, and Sherwood numbers for the droplets have been obtained. Correlations of these numbers with instantaneous Reynolds number and transfer number have been obtained. The flow field has been solved by implicit finite-difference solutions of the Navier-Stokes equations. Explanations for the modifications of lift and drag forces, trajectories, and transport phenomena due to droplet interactions have been formulated. Results have been obtained for fuel droplets, especially in high temperature environments, and, to a limited extent, for liquid oxygen (LOX) droplets in a hot, reducing environment. The results, especially the correlations, should prove useful in spray modelling.

INTRODUCTION

The program on vaporizing droplet interactions in dense sprays has progressed well through its second year. The objectives of the study are to study systematically axisymmetric and three-dimensional interactions amongst droplets in close proximity as found in dense sprays. The transient behavior of fuel droplets and liquid oxygen (LOX) droplets in dense vaporizing sprays is of particular interest. Details of the flow fields and thermochemical fields in the dispersed phase (droplets) and in the continuous phase (gas) are sought. Global properties such as drag coefficients, lift coefficients, moment coefficients, Nusselt numbers, Sherwood numbers, Reynolds numbers, and droplet trajectories are also determined.

The general approach involves implicit finite-difference computations of the unsteady, multidimensional, two-phase flows. On account of moving interfaces, non-Newtonian frames of reference, and widely varying time scales in the two phases, the computations are certainly non-standard and very challenging. Many hundreds of Cray Y-MP hours have been utilized for the calculations. Separate proposals have been written to various NSF Supercomputer Centers in order to acquire these needed CPU hours.

The most interesting and useful results relate to drag modification when droplets are moving in tandem and to drag modification and lift creation when droplets are moving in parallel. These two cases represent the two fundamental types of interactions in a dense spray where droplets are moving in the same general direction. That is, a given droplet is primarily affected by the wake of a droplet ahead of it, and/or by the partial flow blockage resulting from another droplet traveling in parallel alongside of it.

The results of the research are detailed in seven publications listed in the references: Chiang, Raju, and Sirignano (1991), Chiang and Sirignano (1990, 1991a, 1991b), and Kim, Elghobashi, and Sirignano (1991a, 1991b, 1992). A summary of recent progress is presented in the next three sections for each of the three major tasks of the program. The three-dimensional computations have been the largest task. The study on interactive, axisymmetric fuel droplets was basically completed in the first year; only some particular refinements have been required. The third task on interactive LOX droplets has required some special considerations related to near-critical or supercritical behavior.

THREE-DIMENSIONAL DROPLET INTERACTIONS

As a first step toward understanding the three-dimensional interactions in large concentrations of particles, we investigated three-dimensional flow interactions with two identical spheres held fixed relative to each other in the transverse direction against the uniform stream at Reynolds numbers 50, 100, and 150 as shown in Figure 1. We determined the effects of three-dimensional interactions on the lift, moment, and drag coefficients as a function of the dimensionless distance between the two spheres and Reynolds number. In order to understand fully the essential issues, both liquid spheres and solid spheres were investigated. (The following results are for the liquid spheres case.)

We found that, for a given Reynolds number, the two spheres are repelled as the spacing between them becomes of the order of the sphere diameter and, conversely, the two spheres are attracted weakly at intermediate separation distances as shown in Figure 2 (Kim, Elghobashi, and Sirignano 1991a, 1991b). We also found that, for small spacing, the vortical structure of the near wake is perturbed significantly from the axisymmetric situation, and the flow passing through the gap entrains the outer flow near the symmetry plane containing the sphere centers (Kim, Elghobashi, and Sirignano 1991b).

Figures 3(a) and 3(b) display sketches of typical streamlines over one sphere in the x-z symmetry plane containing the sphere centers. The flow-structure ahead of the sphere is such that the streamlines diverge away from the x-y symmetry plane due to the blockage in the gap between the two spheres as they approach the front stagnation region. Also, interesting phenomena in the near wake have been discovered as the gap between the two spheres decreases. When d_0 equals 2, the upper eddy is not formed by the fluid separating on the upper portion of the sphere, but rather by the fluid turning around the lower eddy and detaching from the sphere as shown in Figure 3(a). Furthermore, when d_0 decreases to 1.5, the upper eddy vanishes, and so does the downstream stagnation point as shown in Figure 3(b). These results are in good agreement with the available experimental and numerical studies (Rosfjord 1974; Dandy and Dwyer 1990).

We also have been studying the droplet interactions in more realistic situations where two identical droplets injected into a combustor are moving into a hot and high-pressure gas as shown in Figure 4. The droplets are decelerated, due to the drag, and change their direction of motion, due to the lift. With the origin of a noninertial reference frame at the center of mass of the two droplets, the Navier-Stokes equations can be solved with a noninertial term to be evaluated from Newton's law in an iterative manner.

The moving droplets change their direction due to the interactions. However, a computational grid must be generated such that the lift and torque are zero for a single sphere moving in any direction. We algebraically generate the three-dimensional grids with the above property by using

a group of ellipsoids, cones, and planes, where grid density is controlled by the stretching function developed by Vinokur (1983). Figure 5 represents grid systems on the x-y symmetry plane containing the sphere centers at dimensionless distance $d_o = 7$. Note that the developed numerical scheme is general for arbitrary grid systems so that it is necessary only to change the subroutines of grid generation for more complicated geometries.

To check our three-dimensional code with the new adapting computational grid, we used the code to solve the flow generated by an impulsively started spherical droplet into initially quiescent fluid. With a change of reference to the center of the moving sphere, the problem can also be viewed as an impulsively started flow over a droplet. We relaxed the solution to steady state and compared our results with those from the numerical correlation by Rivkind and Ryskin (1976). The code gives convergent results which agree excellently with the correlation as shown in Table 1, where N_1 , N_2 , and N_3 denote the number of grids in radial (ξ), angular (η), and azimuthal (ζ) directions as shown in Figure 4. Note that η encompasses 90 degrees and ζ encompasses 360 degrees in the physical domain. The calculations were performed for a viscosity ratio (liquid to gas) of 25 and density ratio of 300, which are typical of a liquid-hydrocarbon fuel in a high-temperature, high-pressure surrounding gas generally encountered in gas turbine combustors (Raju and Sirignano 1990). Since the code solves for the Cartesian components of velocity in a transformed grid, an axisymmetric test calculation still exercises the fully three-dimensional aspects of the code.

We have solved the problem of two identical droplets injected in the incompressible fluid medium, initially separated by a distance $d_o = 2$ with no angle of attack at Reynolds number 100. We note that the results below are obtained by using the coarse grid ($20 \times 11 \times 32$).

Figure 6 shows the locus of one droplet for the time period $0 \leq t \leq 300$, where d_t is the instantaneous distance between the spheres and l_t is the instantaneous position in the y direction. It is shown that the droplets are decelerating due to the drag force and repelling due to the lift force, and the repelling is relatively small compared to the deceleration.

Figure 7 shows the histories of the drag coefficients for a single isolated droplet and for the droplet with initial dimensionless distance $d_o = 2$ during the time period $0 \leq t \leq 300$. The drag coefficient of the sphere with $d_o = 2$ is higher than that of a single isolated sphere. Also, the deceleration of the sphere with $d_o = 2$ is higher because of high pressure and shear stress due to the interaction of the spheres.

We are now extending our code to solve the case with the vaporizing droplets injected into a hot and high-pressure environment. We are preparing a paper (Kim, Elghobashi, and Sirignano, 1992) for the 30th AIAA meeting in Reno, Nevada based on the results expected during November and December for the vaporizing droplets problem.

AXISYMMETRIC INTERACTIVE FUEL DROPLET CALCULATIONS

One minor task has been performed in this project since the last annual report. We have conducted several test runs to investigate the grid size dependency on transfer coefficients. The results have indicated that the grid-size dependency becomes significant only for the case with the downstream droplet smaller than the upstream droplet. Hence, we repeated some calculations with small downstream droplets. A slightly modified set of correlations has been obtained. These modest changes will be presented in detail in the revised version of Chiang and Sirignano (1990).

AXISYMMETRIC INTERACTIVE LOX DROPLET CALCULATIONS

We have conducted a detailed analysis of LOX droplet heating and vaporization and the mixing of the oxygen and fuel vapors in a high temperature, low pressure (10--20 atm), convective environment. The effects of variable thermophysical properties, real gas behavior, transient heating and internal circulation of liquid, deceleration of the flow due to the drag of the droplet, boundary-layer blowing, and moving interface are included. A primitive-variable formulation for both gas and liquid phases and an implicit finite-difference scheme have been developed to solve the complete set of Navier-Stokes, energy, and species equations. Some preliminary results have been presented in Chiang and Sirignano (1991b).

We have noticed that most rocket engine combustors are operated in the very high pressure domain where LOX droplets may vaporize under near or even super-critical conditions. Hence, the current objective of this task is concentrated on an understanding of fundamental transport processes underlying high pressure LOX droplet vaporization.

The extension of the present low pressure model to cover the pressure range from the subcritical region to the supercritical region is currently underway. The solubility of the fuel vapor in the liquid phase makes a multicomponent droplet formulation necessary. Also, a new technique is needed to compute mass fraction and thermophysical properties at gas/liquid phase equilibrium and to account for the droplet regression rate due to vaporization as well as phase change across the critical surface, with continuous density and temperature gradients at the surface.

A brief description of the new phase equilibrium conditions at the droplet interface is given below.

Thermodynamic equilibrium of a mixture gives

$$T^l = T^g, \quad P^l = P^g, \quad f_i^l = f_i^g$$

which ultimately presents the following system of equations to be solved:

$$\begin{aligned} x_{O_2}^l \times \phi_{O_2}^l(x_{O_2}^l, x_{H_2}^l, T, P) &= x_{O_2}^g \times \phi_{O_2}^g(x_{O_2}^g, x_{H_2}^g, T, P) \\ x_{H_2}^l \times \phi_{H_2}^l(x_{O_2}^l, x_{H_2}^l, T, P) &= x_{H_2}^g \times \phi_{H_2}^g(x_{O_2}^g, x_{H_2}^g, T, P) \end{aligned}$$

The single-component interface equations are replaced by the following interface equations for a multicomponent fluid.

Conservation of species:

$$\left[\dot{m}_v Y_i - \rho D_{ij} \frac{\partial}{\partial r} Y_i \right]_{r,+} = \left[\dot{m}_v Y_i - \rho D_{ij} \frac{\partial}{\partial r} Y_i \right]_{r,-}$$

Conservation of energy:

$$-\kappa \frac{\partial}{\partial r} T \Big|_{r,-} = \kappa \frac{\partial}{\partial r} T \Big|_{r,+} + \left[\dot{m}_v Y_{O_2} - \rho D_{ij} \frac{\partial}{\partial r} Y_{O_2} \right]_{r,+} (\Delta \bar{H}_{v,O_2} - \Delta \bar{H}_{v,H_2}) + \dot{m}_v \Delta \bar{H}_{v,H_2}$$

where $\dot{m}_v = \rho(V - \dot{r})_{r,+}$

In order to consider real gas effect at high pressure conditions, the ideal gas equation of state is replaced by a Redlich-Kwong equation of state combined with mixing rules. The enthalpy of vaporization is derived from the equation of state by using the fugacity equation.

A phase equilibrium diagram and enthalpy of vaporization from this analysis is given in Figure 8. The available information about the thermophysical and transport properties of fluids under high-pressure conditions, particularly for multicomponent mixtures, has been evaluated and implemented in our existing models.

In parallel to the high-pressure LOX calculation, we are modifying the previous program for the interactive hydrocarbon-fuel droplet to take LOX or hydrogen droplet vaporization into account. The modifications include: (1) a primitive variables approach for liquid phase, (2) thermodynamics property evaluations for oxygen and hydrogen fuel, and (3) more accurate formulation of the interface to include droplet surface expansion.

The three basic configurations include: (1) a LOX droplet following in the wake of another LOX droplet, (2) a LOX droplet following in the wake of a fuel droplet, and (3) a fuel droplet moving in the wake of a LOX droplet. All of the computations are performed for the low pressure case.

We currently are addressing several technical difficulties listed below:

1. There is a need for a suitable initial variable profile to start the calculation. The pressure field (and mass residual sum) between two droplets could destroy solutions since a large magnitude of vaporization occurs if droplets suddenly encounter an inappropriate temperature profile at the beginning of the simulation.

2. The computation will be very costly. The whole primitive variables calculation for a vaporizing LOX or hydrogen droplet requires a very small time step to guarantee a converged solution at the droplet interface. In addition, the grid generation routine requires more iterations to keep track of the rapidly recessing droplet surface.

We will modify the current computational model to improve the numerical stability problem. Also, a simple formulation of droplet vaporization may be constructed in order to conserve our very limited CRAY Y-MP hours. More detailed thermophysical property information for a hydrogen droplet is currently being compiled.

NOMENCLATURE

a_o	dimensional sphere radius
C_D	drag coefficient, $2F_D/\rho U_{\infty,t}^2 \pi a_o^2$
C_L	lift coefficient, $2F_L/\rho U_{\infty,t}^2 \pi a_o^2$
D	center-to-center spacing between two droplets
D_{ij}	binary diffusion coefficient
d_o	initial dimensionless distance between sphere centers normalized by sphere diameter
d_t	instantaneous dimensionless distance between sphere centers
f	fugacity
$\Delta \bar{H}_v$	enthalpy of vaporization
l_t	instantaneous dimensionless moving distance in y direction
\dot{m}_v	mass evaporation rate
N_1	number of grids in ξ direction
N_2	number of grids in η direction
N_3	number of grids in ζ direction
P	pressure
r	radial direction
Re	initial Reynolds number based on sphere diameter, $U_{\infty} 2a_o/\nu$
Re_t	instantaneous Reynolds number, $U_{\infty,t} 2a_o/\nu$
T	temperature
t	dimensionless time normalized by a_o/U_{∞}
U_{∞}	initial dimensional free stream velocity
$U_{\infty,t}$	instantaneous dimensional free stream velocity
x, y, z	Cartesian coordinates
x	mole fraction
Y	mass fraction
ξ, η, ζ	nonorthogonal generalized coordinates
ϕ	fugacity coefficient

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- C. H. Chiang, M. S. Raju, and W. A. Sirignano (1991), Numerical analysis of convecting, vaporizing fuel droplet with variable properties, to appear in *Int. J. Heat Mass Transfer*. Also *AIAA 27th Aerospace Sciences Meeting*, Paper 89-0834 (1989).
- C. H. Chiang and W. A. Sirignano (1990), Numerical analysis of interacting, convecting, vaporizing fuel droplets with variable properties, *AIAA 28th Aerospace Sciences Meeting*, Paper 90-0357. Also submitted to *Int. J. Heat Mass Transfer*.
- C. H. Chiang and W. A. Sirignano (1991a), Axisymmetric calculations of three-droplet interactions, presented at the *Fifth International Conference on Liquid Atomization and Spray Systems*, Gaithersburg, MD U.S.A., July 1991.
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- Kim, I., Elghobashi S. and Sirignano, W. A. (1992), Three-dimensional flow computation for two interacting, moving droplets, *AIAA 30th Aerospace Sciences Meeting*, Paper 92-0343.
- Raju, M. S. and Sirignano, W. A. (1990), Interaction between two vaporizing droplets in an intermediate-Reynolds-number flow, *Phys. Fluids*, **A,2**(10), 1780-1796.
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PUBLICATIONS

The following papers and one book article have resulted at least partially from the research performed under the three tasks of this research program.

1. Raju, M. S. and Sirignano, W. A. (1990), Interaction between two vaporizing droplets in an intermediate-Reynolds-number flow, *Phys. Fluids*, **A,2**(10), 1780-1796.
2. Chiang, C. H., Raju, M. S., and Sirignano, W.A. (1991), Numerical analysis of convecting, vaporizing fuel droplet with variable properties, to appear in *International Journal of Heat and Mass Transfer*. Also see Preprint No. 89-0834, *AIAA 27th Aerospace Sciences Meeting* (1989).
3. Chiang, C. H., and Sirignano, W. A. (1990), Numerical analysis of interacting, convecting, vaporizing fuel droplets with variable properties, submitted to *International Journal of Heat and Mass Transfer*. Also see Preprint No. 90-0357, *AIAA 28th Aerospace Sciences Meeting*.
4. Chiang, C. H., and Sirignano, W. A. (1991), Axisymmetric vaporizing oxygen droplet computations, Preprint No. 91-0281, presented at the *AIAA 29th Aerospace Sciences Meeting*.
5. Chiang, C. H., and Sirignano, W. A. (1991), Axisymmetric calculations of three-droplet interactions, to be submitted to *Atomization and Sprays*. Also presented at the *Fifth International ICLASS Conference on Liquid Atomization and Spray Systems*.

6. Kim, I., Elghobashi, S. E., and Sirignano, W. A. (1991), Three-dimensional flow over two spheres in parallel side-by-side motion, submitted to the *Journal of Fluid Mechanics*. Also see "Three-dimensional droplet interactions in dense sprays", Preprint No. 91-0073 presented at the *AIAA 29th Aerospace Sciences Meeting*.
7. Kim, I., Elghobashi, S. E., and Sirignano, W. A. (1992), Three-dimensional flow computation for two interacting, moving droplets, submitted for presentation at the *AIAA 30th Aerospace Sciences Meeting*.
8. Kim, I., Elghobashi, S. E., and Sirignano, W. A. (1991), Three-dimensional flow interactions between two neighboring spheres, presented at the *44th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*.
9. Sirignano, W. A., Chiang, C. H., Kim, I., and Elghobashi, S. E. (1991), Aerodynamic interactions amongst neighboring droplets, presented at the *4th International Symposium on Computational Fluid Dynamics*.
10. Sirignano, W. A. (1991), Computational challenges in spray combustion, presented at the *U.S.-Japan Heat Transfer Seminar*.
11. Delplanque, J. P., Chiang, C. H., and Sirignano, W. A. (1991), Numerical simulation and modelling of LOX droplet vaporization at supercritical conditions, presented at the *28th JANNAF Combustion Meeting*.
12. Sirignano, W. A., Computational spray combustion, in *Numerical modeling in combustion*, (Chung, T. J., ed.) submitted to Hemisphere Publications, 1990, to appear in 1992.

PROFESSIONAL PERSONNEL

W. A. Sirignano, Professor, Principal Investigator

S. E. Elghobashi, Professor

Kim, I., Postdoctoral Research Associate, Ph.D., January 1990 - present

Chiang, C. H., Postdoctoral Research Associate, September 1990 - present, Ph.D. candidate prior to September 1990

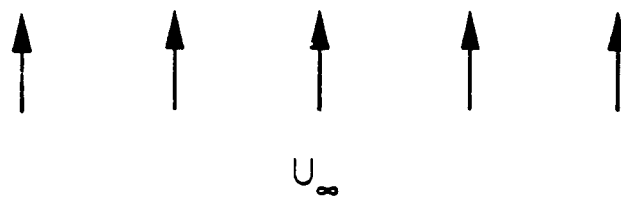
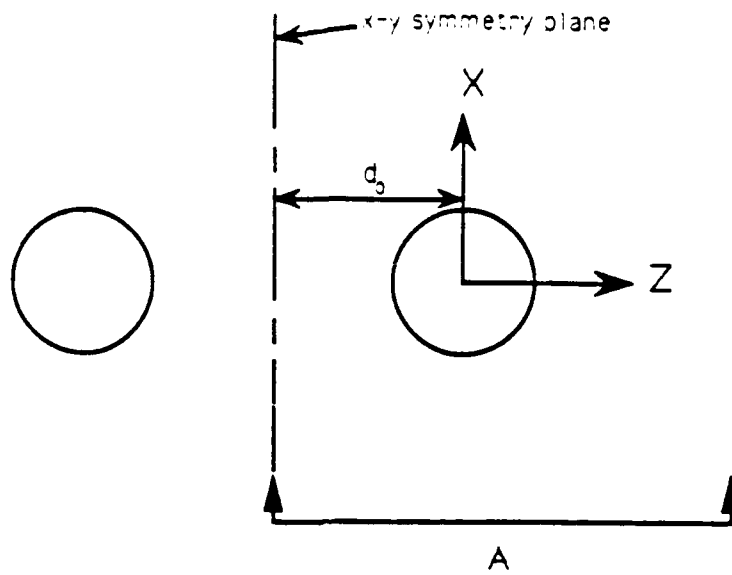
Dissertation Title: Isolated and Interacting, Vaporizing Fuel Droplets: Field Calculation with Variable Properties

INTERACTIONS

Many of the eleven papers listed under publications were presented as conference papers. Even journal papers usually were presented in a precursor form. We have participated in AFOSR Contractors Meetings and Workshops as requested by the sponsor. W. A. Sirignano has served in several advisory or consultant roles with NASA, the National Research Council, and major government contractors. In particular, he has served as: Member, NASA Space Science and Applications Advisory Committee; Member, National Research Council Space Studies Board and Chairman, Committee on Microgravity Research; Consultant, United Technologies Research Center; Consultant, Allison Gas Turbine Division of General Motors; Member, USRA Science Council for Microgravity Science and Applications. Dr. Sirignano has been involved in other research programs funded by AFWAL, AFAL, and ONR that have some relationship to the research performed in this program. Various invited seminars, invited papers or articles, and honors have resulted for the principal investigator based, at least partially, on this AFOSR research. Examples are the 1992 ASME Freeman Scholar Award, which involves a special ASME lecture and journal article, and the 1991 AIAA Pendray Aerospace Literature Award.

$N_1 \times N_2 \times N_3$	$N_{1l} \times N_{2l} \times N_{3l}$	C_{DP}	C_{DV}	C_D	C_D^*
$20 \times 11 \times 32$	$10 \times 11 \times 32$	0.542	0.586	1.128	
$30 \times 15 \times 48$	$15 \times 15 \times 48$	0.520	0.573	1.092	
$40 \times 21 \times 64$	$20 \times 21 \times 64$	0.511	0.571	1.081	1.08

Table 1. Drag coefficients as a function of grid density at $Re = 100$, where * denotes the data from the correlation of Rivkind and Ryskin (1976) and l denotes liquid phase.



view A

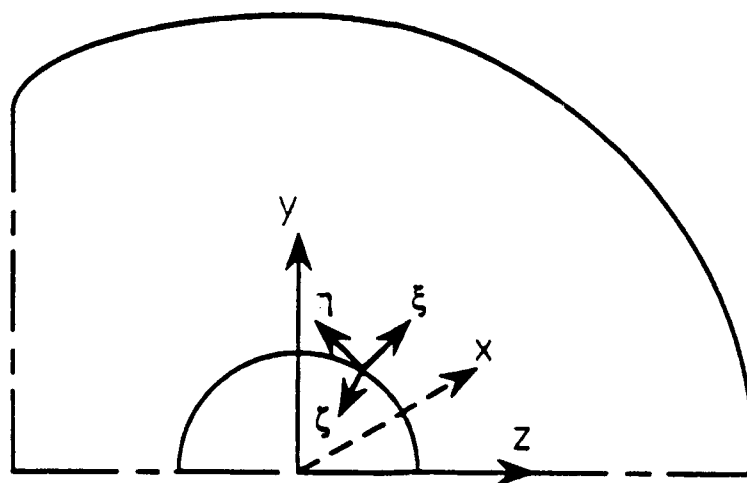


Figure 1. Flow geometry and coordinates.

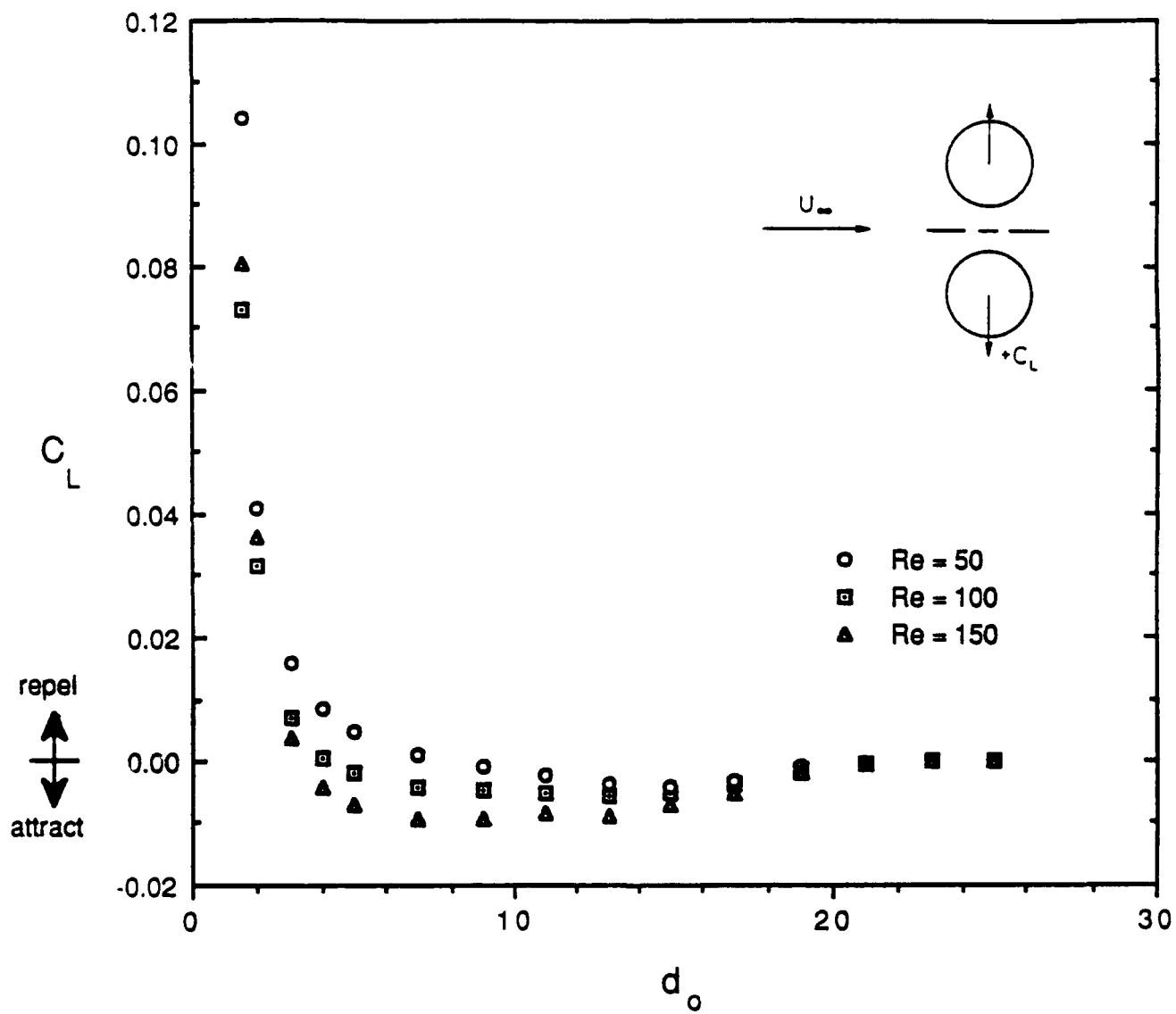


Figure 2. Lift coefficients of liquid sphere as a function of dimensionless distance at $Re = 50, 100$, and 150 .

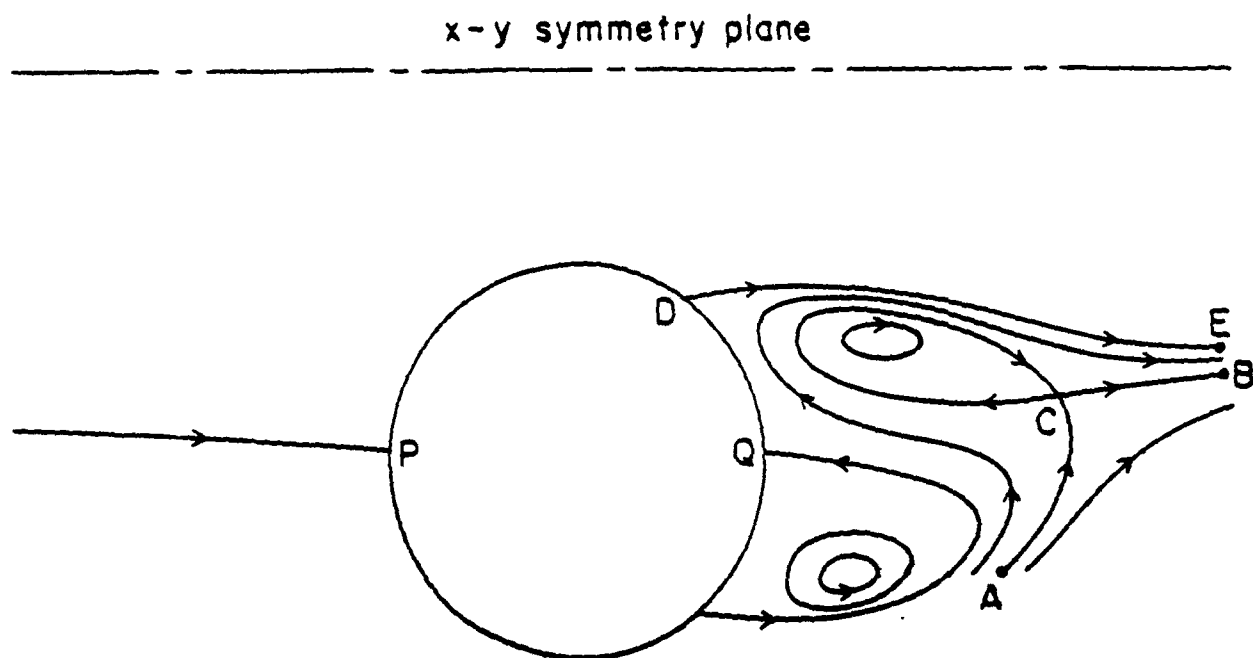


Figure 3(a) Sketch of typical streamlines in the principal plane at $Re = 100$ for dimensionless distance 2.

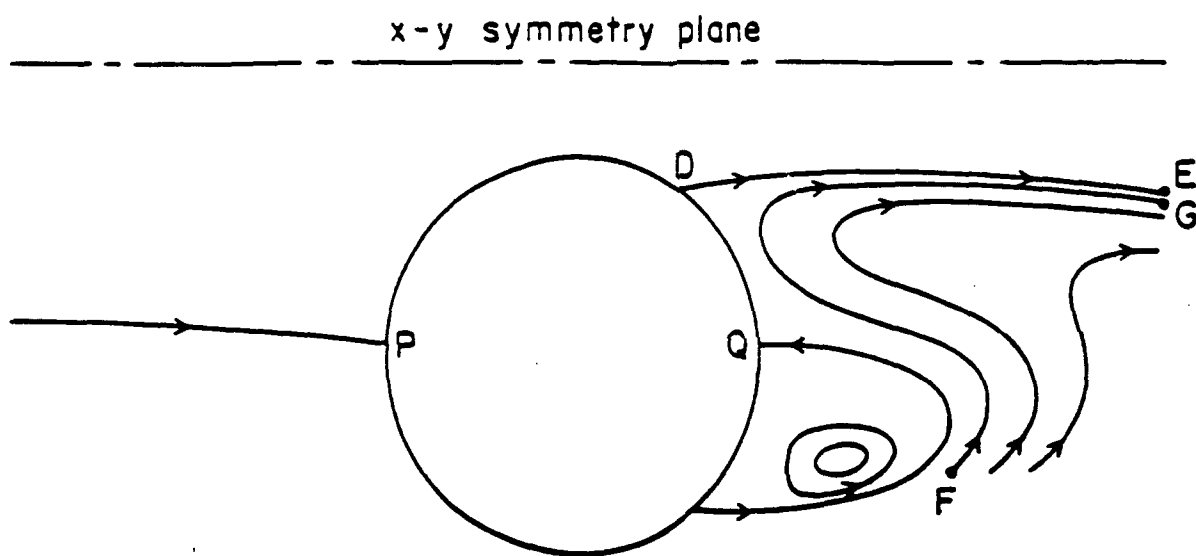
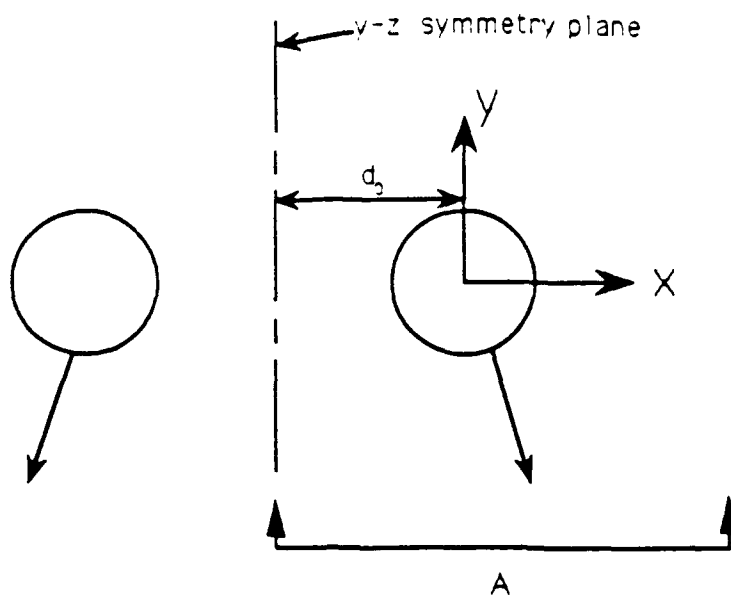


Figure 3(b) Sketch of typical streamlines in the principal plane at $Re = 100$ for dimensionless distance 1.5.



view A

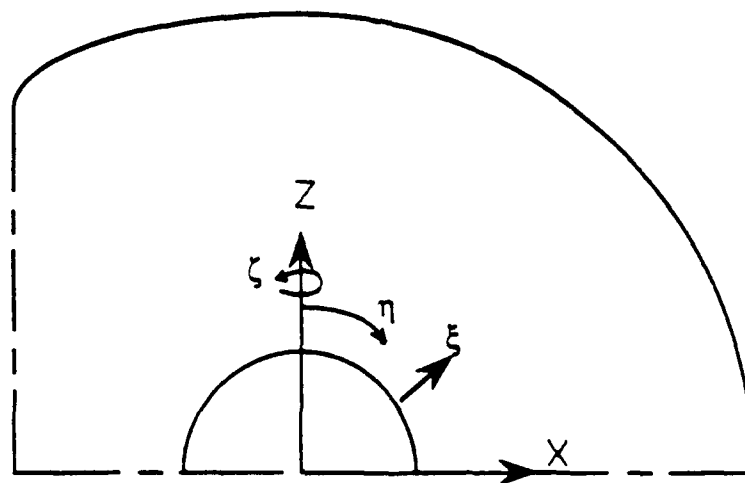


Figure 4. Flow geometry and coordinates

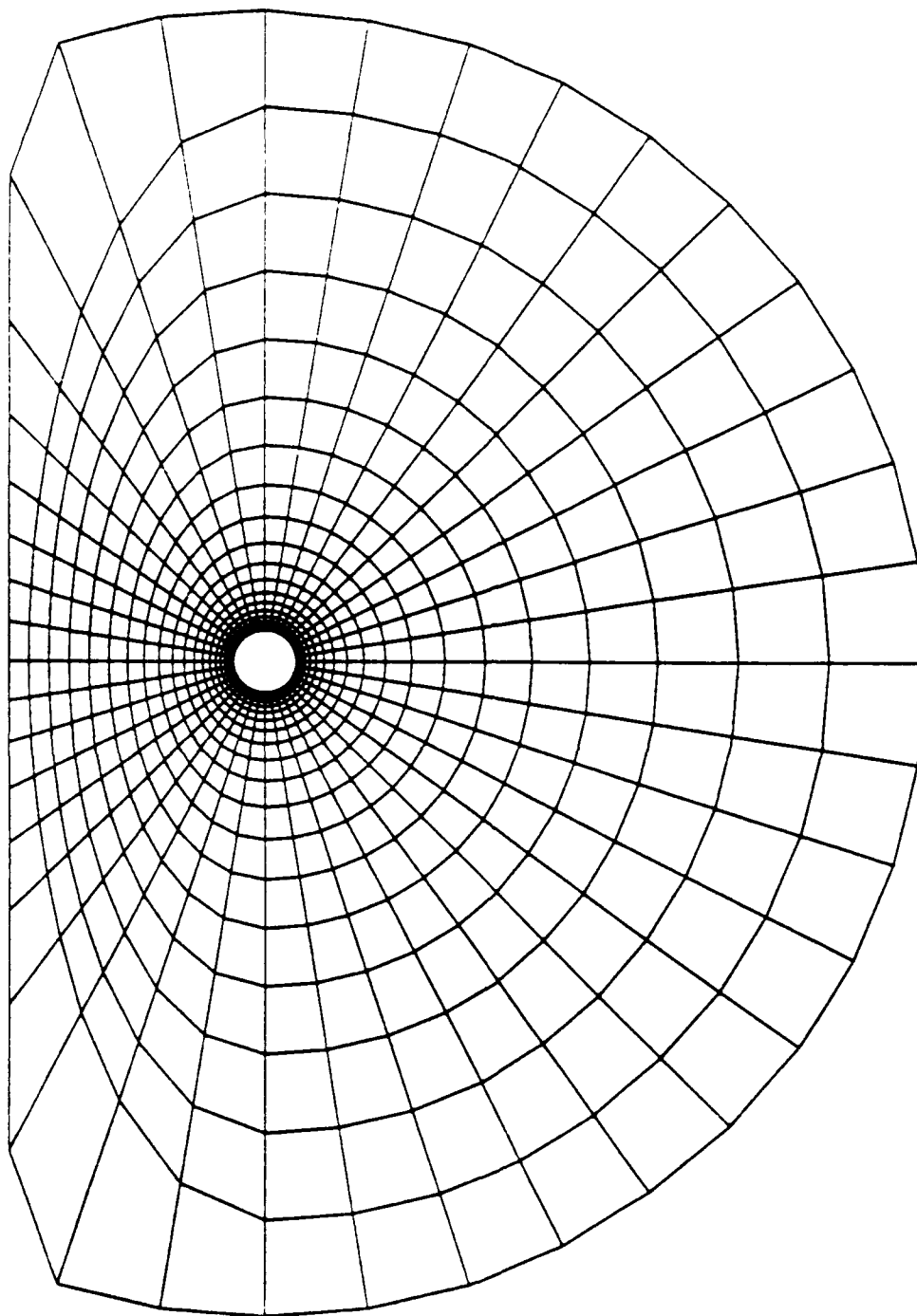


Figure 5. Grid system on x-y plane for dimensionless distance 7.

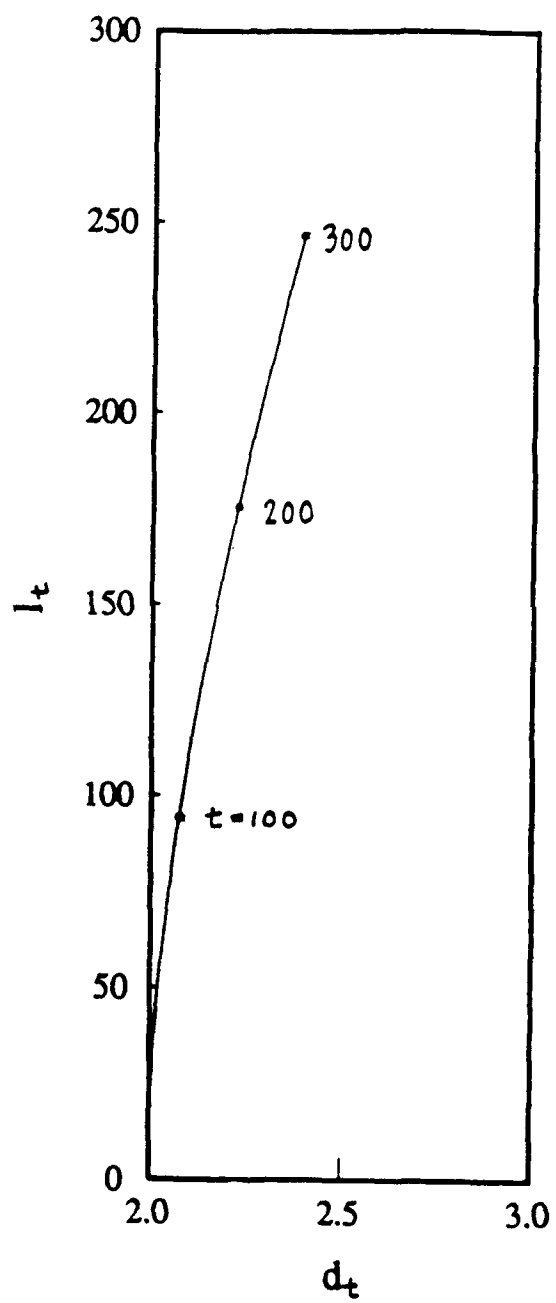


Figure 6. Locus of one droplet for time period $0 \leq \tau \leq 300$.

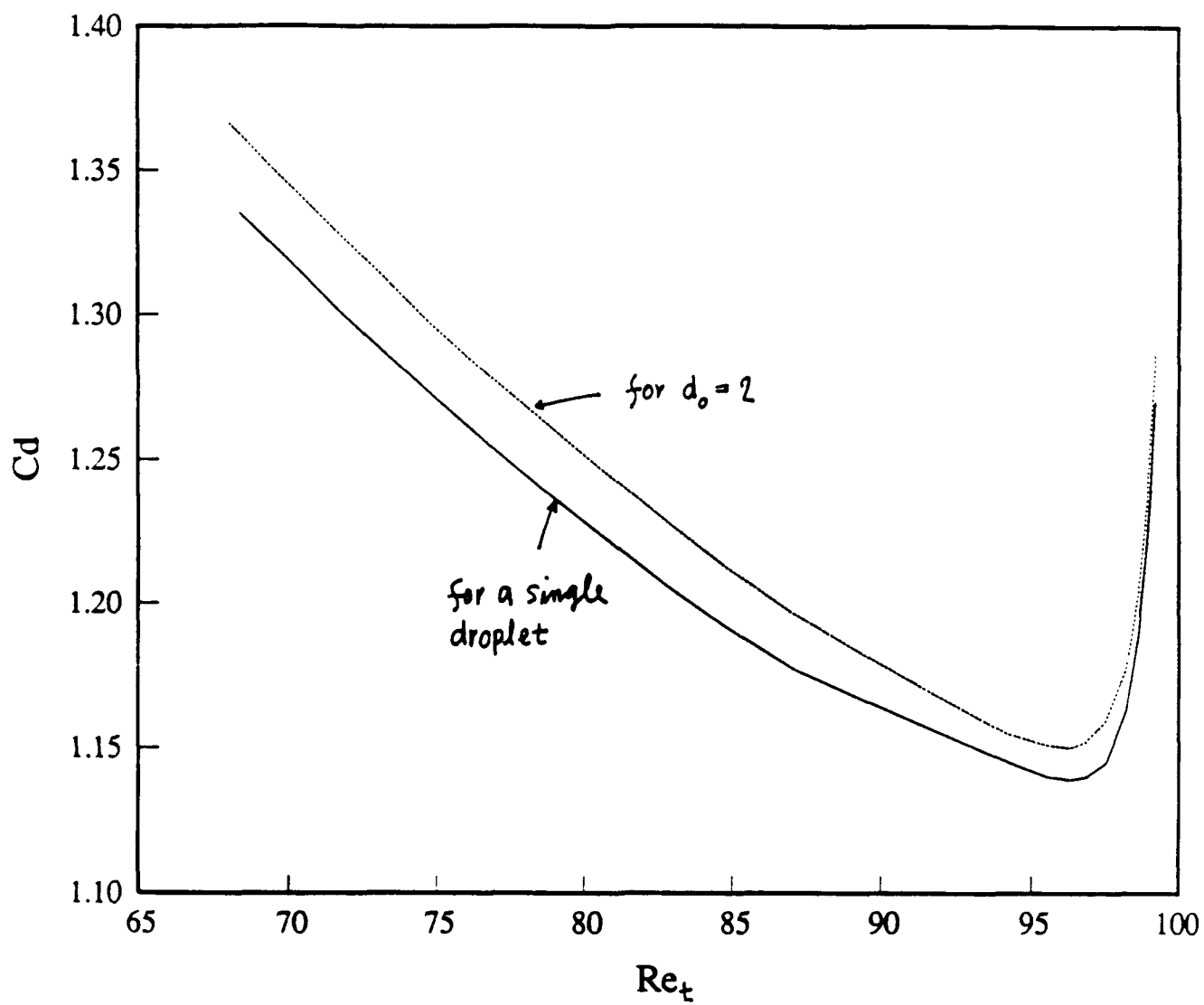


Figure 7. Time variation of drag coefficient for time period $0 \leq t \leq 300$.

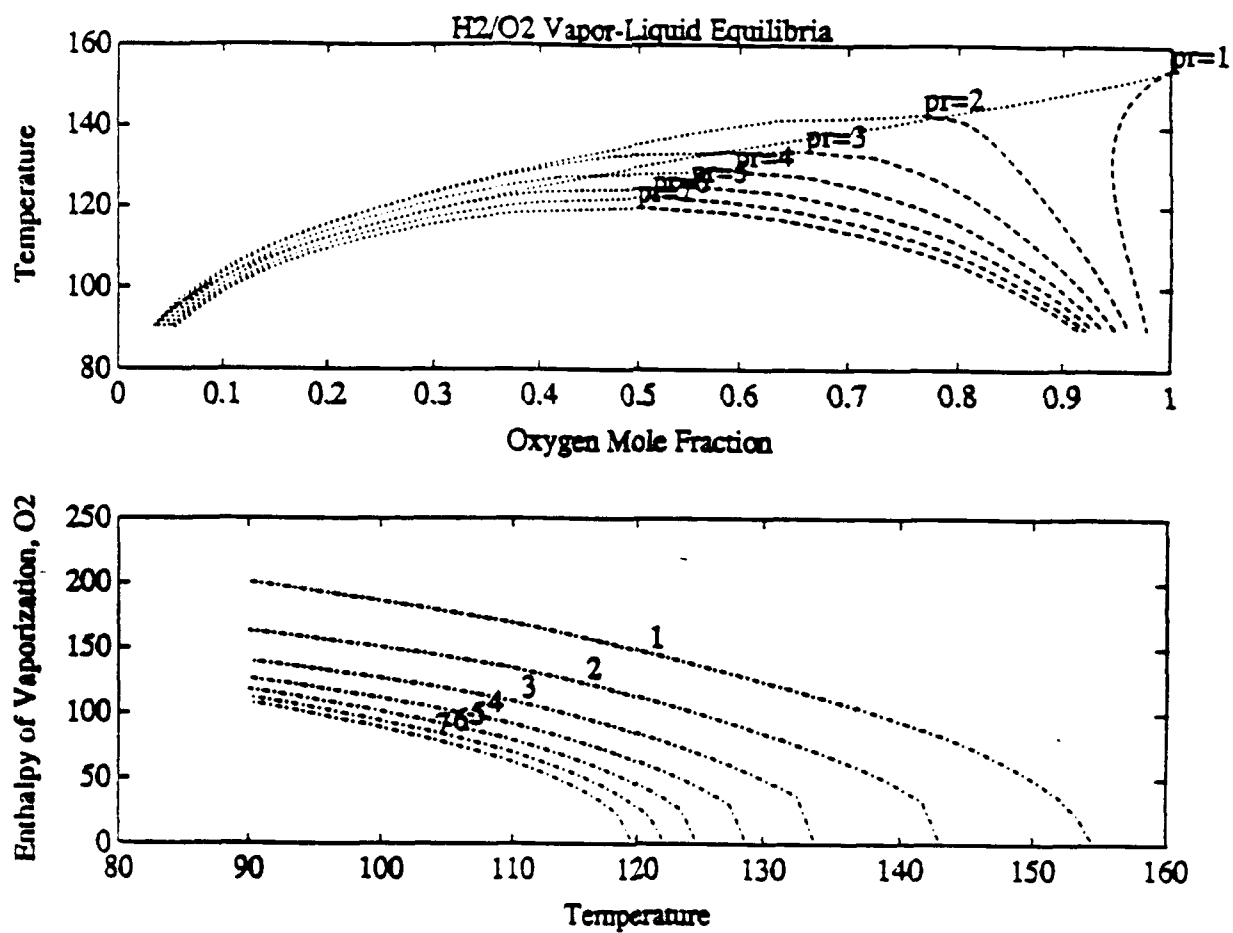


Figure 8. Hydrogen/oxygen vapor-liquid equilibria and enthalpy of vaporization for liquid oxygen at different reduced pressures.